

Testing Continuum and Non-Continuum Descriptions in High Speed Flows

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Abstract. Detailed simulations were performed with a continuum-based Navier-Stokes, a gas kinetic Bhatnagar-Gross-Krook (BGK) and the Direct Simulation Monte Carlo (DSMC) flow solvers to identify and characterize the translational and internal energy mode relaxation in high speed flows. Argon and nitrogen shock structures were simulated to quantify the nonequilibrium state. A new multi-translational temperature gas kinetic model was developed to match the capability of DSMC. Bulk viscosity as an adjustable parameter to recover small departures from rotational equilibrium in the Navier-Stokes equations is explored in weak shock structures. In the context of nitrogen dissociation, the models of vibrational bias for the dissociation kinetics are presented.

INTRODUCTION

The recent resurgence in computing hypersonic viscous/inviscid interactions using Navier-Stokes and DSMC computational methodologies highlights the importance of a unified approach in simulating the translational and internal energy mode relaxation prevalent in such flows. One of the key issues is the ability to use both approaches and obtain consistent solutions for the same flow conditions to hypersonic flow problems that span both the continuum and rarefied flight regimes. The simulation of internal energy mode relaxation is fundamentally different in the two solution approaches. In the continuum approach the Navier-Stokes equations consist of source terms of reaction probabilities for quantifying the thermal and chemical non-equilibrium effects. See for example, Ref. [1]. These are typically available from experiments for equilibrium conditions that have the translational temperature-dependence.

The Navier-Stokes equations, derived from a first order Chapman-Enskog approximation are very successful in hypersonic flows in the continuum regime, typically for a Knudsen number less than 0.1 for small deviations from translational non-equilibrium. However, at higher Knudsen numbers, the microscopic methods based on the Boltzmann equation or the DSMC method provide more detailed information on the degree of non-equilibrium. Equilibrium is established relatively fast for the translational degree of freedom compared to internal degrees of freedom. Usually the gas-kinetic times are small in comparison with the flow times over which appreciable changes in the macroscopic parameters of the gas, density or energy, take place. When these conditions are satisfied it is possible to assign at every instant of time a “translational” temperature, which characterizes the average kinetic energy of translational motion of the particles. However, when the velocity distribution function of the particles is anisotropic, as is the case in low density, hypersonic non-equilibrium flows, multiple translational temperatures, one in the direction of flow and another in the direction perpendicular to the flow, need to be delineated. Detailed simulations were performed in the present study using a continuum-based Navier-Stokes solver, a simplified Boltzmann solver, and a DSMC method to identify and characterize translational and internal energy mode relaxation in high speed flows.

ANALYSIS

The DSMC code is a modified [2, 3] version of that described by Bird [4] suitable for multi-species monatomic and diatomic gas flows. Diatomic molecules are modeled assuming quantized rigid rotor rotational, and anharmonic oscillator vibrational, energy levels. Elastic cross sections are based on the VHS model. Inelastic cross sections (Rotational-Translational and Vibrational-Translational) are based on the Borgnakke-Larsen model assuming constant

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or temperature-dependent collision numbers. Dissociation cross sections are based on the Weak Vibrational Bias model [5], as modified in Ref. [2].

The Boltzmann equation represents the behavior of many-particle kinetic system in terms of the evolution equation for the single particle gas distribution function. The simplified collision model given by Bhatnagar-Gross-Krook (BGK) model formulation is

$$\frac{\partial f}{\partial t} + \mathbf{u} \cdot \frac{\partial f}{\partial \mathbf{x}} = \frac{f^{eq} - f}{\tau} \quad (1)$$

where f , the distribution function, gives the number density of molecules at position \mathbf{x} and velocity \mathbf{u} at time t . If the distribution function f is known, macroscopic variables of the mass, momentum, energy and stress can be obtained by integration over the moments of molecular velocity. In the BGK model, the collision operator involves a simple relaxation to a local equilibrium distribution function f^{eq} with a characteristic time scale τ . Based on the above BGK model, the Navier-Stokes equations can be obtained with the Chapman-Enskog expansion. However, the nonequilibrium effects encountered in the transition to the rarefied flows, such as translational and rotational nonequilibrium, cannot be satisfactorily described in the continuum model, hence, a kinetic description, Eq. 1, becomes necessary. With the modification of the particle collision time, the validity of the kinetic model is extended beyond that of the Navier-Stokes equations. An earlier attempt based on this model was successful for shock structure calculations of the monatomic gas with a single translational temperature [6]. In the following section, the modification to Eq. 1 to formulate a multiple translational temperature model is presented.

Multi-translational temperature modeling

For a gas with different translational temperatures in the x , y , and z directions, an anisotropic distribution is assumed with equilibrium state prevailing in a given direction, and for a one-dimensional flow, written as:

$$g = \rho \left(\frac{\lambda_x}{\pi} \right)^{1/2} \left(\frac{\lambda_y}{\pi} \right)^{1/2} \left(\frac{\lambda_z}{\pi} \right)^{1/2} \exp[-\lambda_x(u-U)^2 - \lambda_y v^2 - \lambda_z w^2], \quad (2)$$

where ρ is the density, U is the macroscopic velocity in the x -direction, and (u, v, w) the components of the particle velocity in the x, y and z directions, respectively. The parameter λ is related to the gas temperature, given by $\lambda_x = \mathcal{M}/2kT_x$, $\lambda_y = \mathcal{M}/2kT_y$ and $\lambda_z = \mathcal{M}/2kT_z$.

The present paper improves on earlier kinetic models for the translational nonequilibrium to overcome the erroneous shock solutions (See for example Ref. [7]). For this purpose, we reconstructed the particle collision process. Starting from the gas distribution function f for a monatomic gas, the particle collisions drive f to g and \bar{g} , instead of from g to \bar{g} alone. During the course of particle collisions, it is difficult to distinguish the process from f to g or from f to \bar{g} . In terms of the particle collision time for translational nonequilibrium, they can be assumed to be the same. Therefore, for the monatomic gas we construct a generalized BGK model for the translational non-equilibrium,

$$f_t + u f_x = \frac{1}{2} \left[\frac{g - f}{\tau} + \frac{\bar{g} - f}{\tau} \right], \quad (3)$$

where f is the real gas distribution function, and g and \bar{g} are the corresponding Maxwellians. Note that the particle collision time τ is related to the local dynamical viscosity μ and pressure p , i.e., $\tau = \mu/p$. The relation between mass ρ , momentum ρU , total energy ρE , and the thermal energy ρE_{y-z} in the y and z directions are

$$W = \begin{pmatrix} \rho \\ \rho U \\ \rho E \\ \rho E_{y-z} \end{pmatrix} = \int \psi f d\mathbf{u} d\xi d\eta,$$

where $\psi = (1, u, \frac{1}{2}(u^2 + v^2 + w^2), \frac{1}{2}(v^2 + w^2))^T$. Since only mass, momentum and total energy are conserved during particle collisions, f and g satisfy the condition

$$\int \frac{1}{2} [(g - f) + (\bar{g} - f)] \psi_\alpha d\mathbf{u} dv dw = S = (0, 0, 0, s)^T, \quad \alpha = 1, 2, 3, 4. \quad (4)$$

The source term s can be still be modeled as $s = \rho R(T_x - T_y)/3\tau$. For any kinetic model with multiple translational temperatures, one basic requirement is that the averaged temperature $T = \frac{1}{3}(T_x + 2T_y)$ in the 1D case should be

the same temperature as the one-temperature gas kinetic model. If we take moments $(u - U)^2, v^2$ and w^2 on the model given by Eq. 3, we can obtain the temperature evolution equations for individual direction. When we add them together and use the condition $3T = T_x + T_y + T_z$, a single equation for the averaged temperature T can be obtained, $(\rho T)_t + (\rho UT)_x = (\rho T^{eq} - \rho T)/\tau$, which is the same temperature evolution equation from a single temperature BGK model, i.e. $f_t + uf_x = (\bar{g} - f)/\tau$. The model given by Eq. 3 is shown to be a valid extension to recover the multiple temperature non-equilibrium from the original BGK because the averaged temperature from the two-temperature model is the same as that from a single temperature model.

In order to test the above model (Eq. 3), the numerical method developed in Ref. [8] is used to solve Eq. 3. For a finite volume method, $W_j^{n+1} = W_j^n + \frac{1}{\Delta x} \int_0^{\Delta t} (F_{j-1/2}(t) - F_{j+1/2}(t))dt + S_j^n \Delta t$, where W_j^n is the cell averaged mass, momentum, total energy, and the thermal energy in y and z directions, and $F_{j+1/2}$ is the corresponding fluxes at a cell interface by solving Eq. 3. Note that Δt is the time step $\Delta t = t^{n+1} - t^n$, and S_j^n is the source term for the thermal energy. The evaluation of the fluxes is based on the gas distribution function f at a cell interface. For the shock structure calculation, due to the smoothness inside the shock layer, the gas distribution function at a cell interface is constructed using the Chapman-Enskog expansion and has the form

$$f = \frac{1}{2}(g + \bar{g}) - \frac{1}{2}\tau[g_t + \bar{g}_t + u(g_x + \bar{g}_x)] + \frac{1}{2}t(g_t + \bar{g}_t) \quad (5)$$

where the g_x and \bar{g}_x can be obtained from the gradients of macroscopic variables, and g_t and \bar{g}_t can be evaluated from the compatibility conditions $\int (g_t + ug_x)\psi_\alpha dudvdw = 0$ and $\int (\bar{g}_t + u\bar{g}_x)dudvdw = 0$. Even with the ability to recover two translational temperatures, the non-equilibrium distribution (Eq. 5) is truncated to the Navier-Stokes order and it will not be accurate in the description of rarefied flow. In order to capture the translational non-equilibrium effect in the rarefied flow regime, the constitutive relationship between viscosity coefficient and other macroscopic variables have to be modified through the generalization of particle collision time [6]. The generalized τ^* will depend not only on the macroscopic variables, but also on their gradients. The basic BGK model does not recover the correct Prandtl number, therefore, to simulate the flow with a realistic Prandtl number, a modification of the heat flux in the energy transport at a cell interface, as used in Ref. [8], is implemented in the current study.

Bulk viscosity and rotational relaxation

A diatomic gas at moderate temperature will experience collisional energy exchange between the translational and (quantized) rotational modes. It is difficult to write the Boltzmann equation in this case. The general model will depend on the assumed molecular shape (viz. spherical).

Based on the quasi-classical theory, Wang Chang and Uhlenbeck [9] carried out the Chapman-Enskog expansion to Navier-Stokes order. With the principal assumption of short relaxation times and the same temperature to describe the translational and rotational energy modes, they derived the pressure tensor in the Navier-Stokes equations as

$$p_{ij} = p^* - \eta \frac{\partial U_k}{\partial x_k} \delta_{ij} - \mu \left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) \quad (6)$$

where p^* is the equilibrium pressure, μ the shear viscosity coefficient, and η the bulk viscosity coefficient. The practical importance of bulk viscosity depends on the relative magnitudes of μ and η . Lighthill [10] obtained the same result, where the bulk viscosity is expressed as $\eta = (\gamma - 1)^2 \rho e^{\frac{c_{vrot}}{c_v}} \bar{\tau}$ where $\bar{\tau}$ is the mean relaxation time for the rotational energy, which is usually written as $\bar{\tau} = Z_R \tau$ and τ is the collision time and Z_R is the rotational collision number.

In the long relaxation limit, Wang Chang and Uhlenbeck derived an equation which in essence is the Navier-Stokes equations with an additional relaxation equation for the internal energy. This equation set has no additional bulk viscosity term in the stress tensor since the dissipation due to rotational relaxation is explicitly accounted for with the relaxation equation below, an equation also known as Jean's equation.

$$\rho \frac{De_r}{Dt} - \frac{\partial}{\partial x_i} \kappa_r \frac{\partial T_r}{\partial x_i} = \rho \frac{e_r^{eq}(T_t) - e_r}{Z_R \tau} \quad (7)$$

The usage of the two limiting equations mentioned above depends on whether the relaxation process has the short or long relaxation time. More specifically, the criteria [11] can be expressed as $\omega\tau = \tau/\delta t$, where δt is the characteristic time scale. For the sound wave propagation, the condition $\omega\tau \simeq l/\lambda \ll 1$ can be satisfied when the wavelength

of the sound wave λ is much larger than the mean free path of the particle collision. However, for the shock wave structure, $\omega\tau \simeq M/N$, where M is the Mach number and N is the number of mean free paths inside the shock layer; the characteristic time being the time for a particle to pass through the shock layer. Therefore, the bulk viscosity equations are not suitable for studies of strong shock waves. The relaxation models are more suitable for shock structure computations and as noted later in the results section, the bulk viscosity modifications can provide reasonable predictions for weak shock structures.

Dissociation Kinetics

With an increase in flow velocity (or temperature), collisional energy (translational and internal) becomes sufficient to initiate dissociation in diatomic molecules. The dissociation process in the continuum formulation is modeled in the form of an Arrhenius equation $k_f(T_{\text{eff}}) = C_f T_{\text{eff}}^\eta \exp(\theta_d/T_{\text{eff}})$ where the rate controlling temperature, T_{eff} requires an appropriate definition. Present day hypersonic codes have often used the Park model to define the rate controlling dissociation temperature, due to its ease of implementation. However, the model is shown to be inaccurate for a wide range of temperatures. In order to highlight the kinetic implications of nonequilibrium relaxation, dissociation models differing in the vibrational bias, suitable for a wide range of degrees of nonequilibrium are discussed.

The Park model [12] expresses the dissociation coefficient in terms of an effective temperature: $T_{\text{eff}} = \sqrt{TT_v}$ and $k_{d,\text{eff}} = k_{d,\text{eq}}(T_{\text{eff}})$. The Ladder and Weak Bias model were developed considering the energy in the vibrational quantum states of the dissociating diatomic molecule. Dissociation in the Ladder model is assumed to take place only from the last bound state whereas for the Weak Bias model *all* quantum states contribute. The dissociation rate of the Ladder model can be written as, $n_v^* k_{v^* \rightarrow \text{Continuum}}$ where, n_v^* is the vibrational population in the last state and $k_{v^* \rightarrow \text{Continuum}}$ is the dissociation rate from the last vibrational state. The Weak Bias model, in contrast to the previous model, assumes dissociation to proceed from all the states, viz. $n_0 k_{0 \rightarrow \text{Continuum}}$, $n_1 k_{1 \rightarrow \text{Continuum}}$, $n_2 k_{2 \rightarrow \text{Continuum}}$ and so on to $n_v^* k_{v^* \rightarrow \text{Continuum}}$.

In order to facilitate a comparison of the global rate of dissociation under different conditions of vibrational bias, it is useful to define an effective dissociation rate, $k_{d,\text{eff}}[T, T_v]$, where: $k_{d,\text{eff}}[T, T_v] N_{\text{tot}} \equiv \sum_{v=0}^{v^*} k_{d_v} n_v$ and k_{d_v} is the dissociation coefficient from vibrational state v and is assumed to be a function of T only. By expressing the functional dependence of the population in each vibrational state in terms of a vibrational temperature: $n_v = \frac{N_{\text{tot}} \exp(-\frac{\epsilon_v}{kT_v})}{Z_{\text{vib}}}$ where Z_{vib} is the vibrational partition function, ϵ_v is the vibrational energy in the quantum level v , k is the Boltzmann constant, N_{tot} is the total number density, and T_v is the vibrational temperature, one can express the $k_{d,\text{eff}}[T, T_v]$ for the Ladder and Weak-Bias model in terms of the equilibrium coefficient $k_d[T]$. For the Ladder model,

$$k_{d,\text{eff}}[T, T_v] = k_{d_{v^*}} \frac{n_{v^*}}{N_{\text{tot}}} = k_{d_{\text{eq}}}[T] \frac{n_{v^*}}{n_{v_{\text{eq}}}} = k_{d_{\text{eq}}}[T] \exp[\epsilon_{v^*}(\frac{1}{T} - \frac{1}{T_v})] \frac{Z_{\text{vib}}[T]}{Z_{\text{vib}}[T_v]}. \quad (8)$$

The Weak Bias form is given by:

$$k_{d,\text{eff}}[T, T_v] = \frac{k_{d_{\text{eq}}}[T]}{(v^* + 1)} \frac{Z_{\text{vib}}[T]}{Z_{\text{vib}}[T_v]} N_{\text{tot}} \sum_{v=0}^{v^*} \exp[\epsilon_v(\frac{1}{T} - \frac{1}{T_v})]. \quad (9)$$

The value of $k_{d_{\text{eq}}}$ is obtained from experiments. Note that nonequilibrium values of the effective dissociation coefficient for the Ladder and Weak Bias forms differ substantially. The state-specific dissociation rates compete with the V-V and V-T rates and the state populations are depleted [13] in the excitation phase.

RESULTS AND CONCLUSIONS

A comparison of solutions of DSMC and a multi-translational temperature gas kinetic model, Fig. 1, are shown for the density and multi-translational temperatures in a Mach 2 argon shock structure. The gas kinetic model predictions of multi-translational temperatures and density (Fig. 1a) have an excellent match with those of DSMC. The averaged, single translational temperature and density predictions (Fig. 1b) and the normal stress and heat transfer predictions (Fig. 1c) of the gas kinetic model match those obtained from the direct solution of the Boltzmann equation [14]. For the case of the Mach 1.2 Argon shock structure, (figure not shown) the macroscopic values of density, temperature, normal stress and heat flux predicted by NS solver match those of DSMC and the direct Boltzmann solutions of Ref. [14]. For

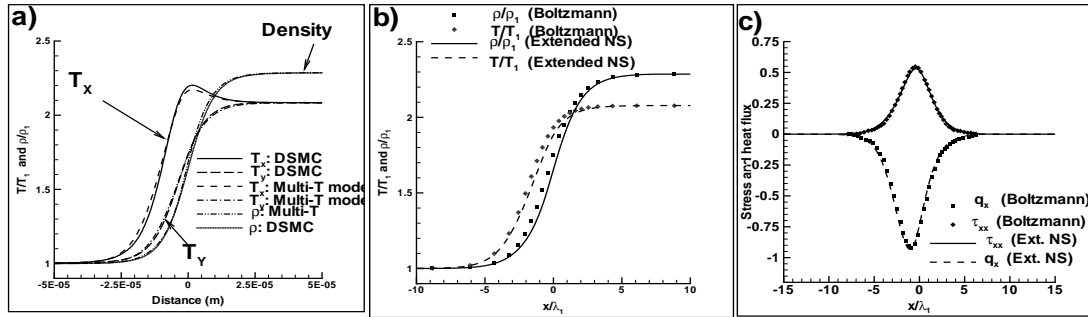


FIGURE 1. Comparison of Mach 2 Argon shock structure, (a) comparison of density and temperature with DSMC, (b) comparison of density and temperature with Boltzmann solution, (c) comparison of stress and heat transfer with Boltzmann solution

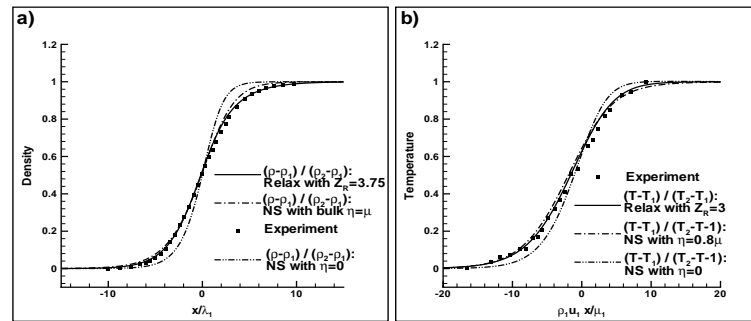


FIGURE 2. Demonstration of bulk viscosity as a rotational relaxation parameter, (a) Mach 1.53 nitrogen shock structure comparison with experiment, (b) Mach 1.9 air shock structure comparison with experiment

higher Mach numbers, however, the NS equations are not adequate and a gas kinetic approach is necessary. For a Mach 2 Argon shock structure shown in this report, the multi-translational temperature, gas kinetic BGK model proposed in this study provides excellent match with the DSMC and direct solutions of the Boltzmann equation [14].

Fig. 2 shows the effect of the variation of the bulk viscosity (to deviate from the Stokes hypothesis) in the Navier-Stokes equation as an alternate means to the explicit modeling of the rotational relaxation inside the shock structure. The predictions are shown for both bulk viscosity variation of $\eta = 0$ and a higher η in the NS equations and for explicit modeling of rotational relaxation by the inclusion of the relaxation parameter, Z_R . Comparisons of NS solutions with bulk viscosity modification with experiment, Fig. 2a shows the improved prediction of density with $\eta = \mu$ for a Mach 1.53 nitrogen shock structure and improved prediction of temperature with $\eta = 0.8\mu$ for a Mach 1.9 air shock structure. It may be concluded that adjusting bulk viscosity in NS equations to model the rotational relaxation is justified for weak shock structures where the values of $\omega\tau \simeq l/\lambda < 1$ and as noted earlier, the relaxation model may be more suitable for strong shock wave structures.

The details of the nonequilibrium dissociation process in a gas are still the subject of research. Various theoretical and phenomenological arguments suggest that the vibrational state or energy of a molecule has a relatively larger influence on its probability of dissociation compared to, e.g., the relative translational energy, or rotational state. In the limiting case, known as the Ladder model in continuum studies, a molecule can dissociate only if it is in the top bound level. Other continuum models may base the rate constant on the geometric mean of the vibrational and translational temperature (energy content) of the gas (e.g., the Park model), or provide for some vibrational bias. Similarly various models, with varying [2] levels of physical realism, have been proposed for treatment of dissociation events at the molecular level, as required in DSMC. The phenomenological weak vibrational bias (WVB) model of Koura [5] has been found to predict basic features of vibrational favoring.

To analyze the dissociation event directly, it is useful to consider as a model problem a spatially uniform, but multi-temperature, bath gas. Fig. 3a shows the calculated two-temperature dissociation rate constant $k_d(T_i, T_v)$ for the case of a nitrogen bath maintained at $T_i = 10,000\text{K}$ as a function of $T_v \leq T_i$. This represents the basic condition that arises

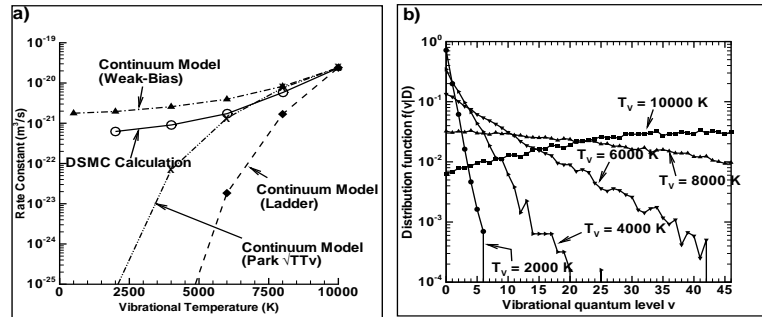


FIGURE 3. Vibrational bias in nitrogen gas at 10,000K, (a) Continuum and DSMC models of bias for different vibrational temperatures, (b) DSMC simulation of the vibrational energy distribution function

in shock layer compression flows, where the internal mode temperature rise lags that of translational temperature, due to the lower inelastic relaxation rates. The DSMC and NS results have been calibrated to recover the same equilibrium rate constant at $T = T_t = T_v = 10,000$ K. The DSMC results use the WVB model, as implemented in Ref. [3], while several continuum dissociation models are shown: Ladder, weak-bias and Park model. The Ladder and Park model exhibit several orders of magnitude lower dissociation rate than the weak bias models. Rich, et al. [15] qualitatively describe the relative influence of vibrational excitation (energy content) on the dissociation behavior of a gas. For assessment of nonequilibrium dissociation phenomena at the microscopic scale, the vibrational distribution function of molecules selected to dissociate, $f(v|D)$, has been found useful. Fig. 3b shows the vibrational energy distribution function of molecules selected for dissociation corresponding to the conditions of Fig. 3a, as predicted by DSMC. As the average vibrational energy content of the gas decreases, molecules in the lower vibrational levels provide the dominant contribution to the overall dissociation rate. Note that each distribution has been independently normalized to obtain $\sum_v f(v|D) = 1$; comparison with Fig. 3a shows that the absolute dissociation rate of the DSMC calculated results decreases by an order of magnitude over the range of vibrational temperature considered here. Models which do not account for this physical effect cannot reproduce this phenomenon over the range of conditions expected in and across a shock wave.

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